COSMOS Workshop, École des Ponts ParisTech

Sharp estimates on metastable lifetimes for one- and two-dimensional Allen–Cahn SPDEs

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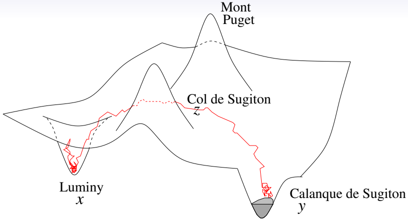
Joint works with Barbara Gentz (Bielefeld),
and with Giacomo Di Gesu (Paris) and Hendrik Weber (Warwick)

Metastability for finite-dimensional SDEs

$$\mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

$V : \mathbb{R}^d \to \mathbb{R}$ confining potential

$\tau_y^x = \inf\{t > 0 \colon x_t \in \mathcal{B}_\varepsilon(y)\}$
first-hitting time of small ball $\mathcal{B}_\varepsilon(y)$,
when starting in x



Metastability for finite-dimensional SDEs

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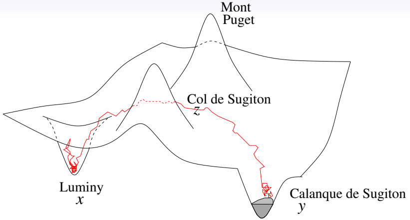

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Arrhenius' law (1889): $\mathbb{E}[\tau_y^x] \simeq e^{[V(z)-V(x)]/\varepsilon}$

Eyring–Kramers law (1935, 1940):
Eigenvalues of Hessian of V at minimum x: $0 < \nu_1 \leqslant \nu_2 \leqslant \dots \leqslant \nu_d$
Eigenvalues of Hessian of V at saddle z: $\lambda_1 < 0 < \lambda_2 \leqslant \dots \leqslant \lambda_d$

$$\mathbb{E}[\tau_y^x] = 2\pi\sqrt{\frac{\lambda_2 \dots \lambda_d}{|\lambda_1|\nu_1 \dots \nu_d}}\,e^{[V(z)-V(x)]/\varepsilon}\big[1 + \mathcal{O}_\varepsilon(1)\big]$$

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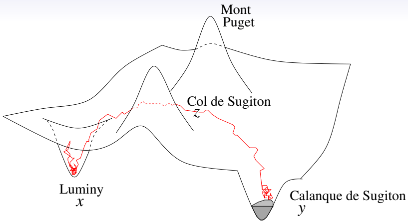

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Arrhenius' law: proved by Freidlin, Wentzell (1979) using large deviations
Eyring–Kramers law: Bovier, Eckhoff, Gayrard, Klein (2004) using potential theory, Helffer, Klein, Nier (2004) using Witten Laplacian, ...

Potential-theoretic proof

"Magic" formula: for $A, B \subset \mathbb{R}^d$ disjoint sets,

$$\boxed{\mathbb{E}^{\nu_{A,B}}[\tau_B] = \frac{1}{\operatorname{cap}_A(B)} \int_{B^c} h_{A,B}(y)\, e^{-V(y)/\varepsilon}\, dy}$$

- Equilibrium measure: $\nu_{A,B}$ proba measure concentrated on ∂A
- Committor function: $h_{A,B}(y) = \mathbb{P}^y\{\tau_A < \tau_B\}$
- Capacity: $\operatorname{cap}_A(B) = \varepsilon \int_{(A\cup B)^c} \|\nabla h_{A,B}(y)\|^2 e^{-V(y)/\varepsilon}\, dy$

  Property: $\operatorname{cap}_A(B) = \varepsilon \inf_{h\in H^1, h|_A=1, h|_B=0} \int_{(A\cup B)^c} \|\nabla h(y)\|^2 e^{-V(y)/\varepsilon}\, dy$

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Proving Eyring–Kramers formula: A and B small sets around x and y

- Variational arguments: $\operatorname{cap}_A(B) \simeq \varepsilon \sqrt{\frac{|\lambda_1|}{2\pi\varepsilon}} \sqrt{\frac{(2\pi\varepsilon)^{d-1}}{\lambda_2 \dots \lambda_d}}\, e^{-V(z)/\varepsilon}$
- Laplace asymptotics: $\int_{B^c} h_{A,B}(y)\, e^{-V(y)/\varepsilon}\, dy \simeq \sqrt{\frac{(2\pi\varepsilon)^d}{\nu_1 \dots \nu_d}}\, e^{-V(x)/\varepsilon}$
- Use Harnack inequalities to show that $\mathbb{E}^{\nu_{A,B}}[\tau_B] \simeq \mathbb{E}^x[\tau_B]$

Deterministic Allen–Cahn PDE

[Chafee & Infante 74, Allen & Cahn 75]

$$\boxed{\partial_t u(x,t) = \partial_{xx} u(x,t) + f(u(x,t))}$$

- $x \in [0, L]$
- $u(x,t) \in \mathbb{R}$
- Either periodic or zero-flux Neumann boundary conditions
- In this talk: $f(u) = u - u^3$ (results more general)

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Energy function:

$$V[u] = \int_0^L \Big[\frac{1}{2}u'(x)^2 - \frac{1}{2}u(x)^2 + \frac{1}{4}u(x)^4\Big]\mathrm{d}x \qquad \to \quad \text{min}$$

Scaling limit of particle system with potential

$$V(y) = \frac{N^2}{2L^2}\sum_{i=1}^N (y_{i+1} - y_i)^2 + \sum_{i=1}^N \Big[-\frac{1}{2}y_i^2 + \frac{1}{4}y_i^4\Big]$$

Stationary solutions: $u_0''(x) = -u_0(x) + u_0(x)^3 \qquad$ critical points of V

Stationary solutions

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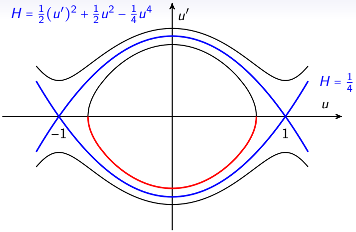
- $u_0(x) \equiv 0$
- Nonconstant solutions satisfying b.c. (expressible in terms of Jacobi elliptic fcts)



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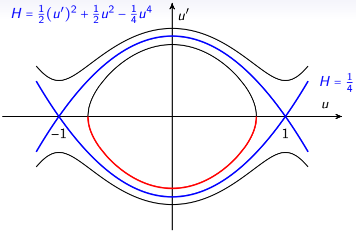

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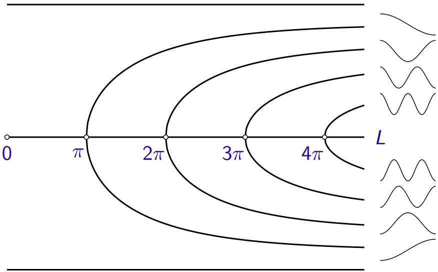
- Neumann b.c: k nonconstant solutions when $L > k\pi$



- Periodic b.c: k families when $L > 2k\pi$

Stability of stationary solutions

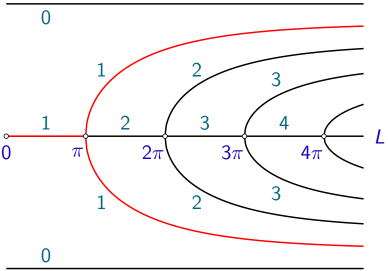
$u_0''(x) = -u_0(x) + u_0(x)^3$

Variational eq around u_0: $\partial_t v_t(x) = v_t''(x) + [1 - 3u_0(x)^2]v_t(x)$

Sturm–Liouville spectrum of RHS determines stability of u_0

- $u_\pm \equiv \pm 1$: always stable (global minima of V)
- $u_0 \equiv 0$: always unstable, eigenvalues $\lambda_k = \left(\frac{\beta k\pi}{L}\right)^2 - 1$ (Neumann b.c.: $\beta = 1$, periodic b.c.: $\beta = 2$)

Neumann b.c.:
Number of positive eigenvalues (= unstable directions)
Transition state



Coarsening dynamics

[Carr & Pego 89, Chen 04] (Link to simulation)

Stochastic partial differential equations

$$\dot{u}_t(x) = \Delta u_t(x) + f(u_t(x)) \quad + \sqrt{2\varepsilon}\, \ddot{W}_{tx} \qquad (\Delta \equiv \partial_{xx}, f(u) = u - u^3)$$

$\ddot{W}_{tx}$: space–time white noise (formal derivative of Brownian sheet)

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Construction of mild solution via Duhamel formula:

- $\dot{u}_t = \Delta u_t \qquad \Rightarrow \qquad u_t = \mathrm{e}^{\Delta t}\, u_0$
  where $\mathrm{e}^{\Delta t}\cos\big(\frac{k\pi x}{L}\big) = \mathrm{e}^{-(k\pi/L)^2 t}\cos\big(\frac{k\pi x}{L}\big)$

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$$w_t(x) = \sum_k \int_0^t \mathrm{e}^{-(k\pi/L)^2(t-s)}\, \mathrm{d}W_s^{(k)} \cos\left(\frac{k\pi x}{L}\right) \in H^s \cap \mathcal{C}^\alpha \ \forall s, \alpha < \frac{1}{2}$$

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$$\Rightarrow \qquad u_t = \mathrm{e}^{\Delta t}\, u_0 + \sqrt{2\varepsilon}\, w_t + \int_0^t \mathrm{e}^{\Delta(t-s)}\, f(u_s)\, \mathrm{d}s =: F_t[u]$$

$\Rightarrow$ Existence and a.s. uniqueness [Faris & Jona-Lasinio 1982]

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Fourier variables: $u_t(x) = \frac{1}{\sqrt{L}} \sum_{k=-\infty}^{\infty} z_k(t)\, \mathrm{e}^{\mathrm{i}\pi kx/L}$

$$\Rightarrow \qquad \mathrm{d}z_k = -\lambda_k z_k\,\mathrm{d}t - \frac{1}{L} \sum_{k_1+k_2+k_3=k} z_{k_1} z_{k_2} z_{k_3}\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t^{(k)}$$

Itō SDE, $\mathrm{d}W_t^{(k)}$: independent Wiener processes
$\lambda_k = -1 + (\pi k/L)^2$

Energy functional:

$$V[u] = \frac{1}{2} \sum_{k=-\infty}^{\infty} \lambda_k |z_k|^2 + \frac{1}{4L} \sum_{k_1+k_2+k_3+k_4=0} z_{k_1} z_{k_2} z_{k_3} z_{k_4}$$

$$\Rightarrow \qquad \mathrm{d}z_t = -\nabla V(z_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

Coarsening dynamics with noise

(Link to simulation)

Eyring–Kramers law for 1D SPDEs: heuristics

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Initial condition: $u_{\rm in}$ near $u_- \equiv -1$ with eigenvalues ν_k

Target: $u_+ \equiv 1$, $\tau_+ = \inf\{t > 0\colon \|u_t - u_+\|_{L^\infty} < \rho\}$

Transition state: ($\beta = 1$ for Neumann b.c., $\beta = 2$ for periodic b.c.)

$$u_{\rm ts}(x) = \begin{cases} u_0(x) \equiv 0 & \text{if } L \leqslant \beta\pi \quad \text{with ev } \lambda_k = (\frac{\beta k\pi}{L})^2 - 1 \\ u_1(x) \ \beta\text{-kink stationary sol.} & \text{if } L > \beta\pi \quad \text{with ev } \lambda'_k \end{cases}$$

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[Faris & Jona-Lasinio 82]: large-deviation principle

$\Rightarrow$ Arrhenius law: $\mathbb{E}^{u_{\rm in}}[\tau_+] \simeq e^{(V[u_{\rm ts}] - V[u_-])/\varepsilon}$

[Maier & Stein 01]: formal computation; for Neumann b.c.

$\Rightarrow \mathbb{E}^{u_{\rm in}}[\tau_+] \simeq 2\pi \sqrt{\frac{1}{|\lambda_0|\nu_0} \prod_{k=1}^\infty \frac{\lambda_k}{\nu_k}}\, e^{(V[u_{\rm ts}] - V[u_-])/\varepsilon}$

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- ▷ Rigorous proof?
- ▷ What happens when $L \to \beta\pi$ as then $\lambda_1 \to 0$?

Eyring–Kramers law for 1D SPDEs: main result

Theorem: Neumann b.c. [B & Gentz, Elec J Proba 2013]

▷ If $L < \pi - c$ with $c > 0$, then

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- If $L > \pi + c$, then same formula with extra factor $\frac{1}{2}$ (since 2 saddles) and λ'_k instead of λ_k
- If $\pi - c \leqslant L \leqslant \pi$, then

$$\mathbb{E}^{u_{\rm in}}[\tau_+] = 2\pi \sqrt{\frac{\lambda_1 + \sqrt{3\varepsilon/2L}}{|\lambda_0|\nu_0\nu_1} \prod_{k=2}^{\infty} \frac{\lambda_k}{\nu_k}}\, \frac{\mathrm{e}^{(V[u_{\rm ts}]-V[u_-])/\varepsilon}}{\Psi_+(\lambda_1/\sqrt{3\varepsilon/2L})}\bigl[1 + R(\varepsilon)\bigr]$$

  where Ψ_+ explicit, involves Bessel function $K_{1/4}$, $\lim_{\alpha\to\infty}\Psi_+(\alpha) = 1$
- If $\pi \leqslant L \leqslant \pi + c$, then same formula, with another function Ψ_-, involving Bessel functions $I_{\pm 1/4}$, $\lim_{\alpha\to\infty}\Psi_-(\alpha) = 2$

Eyring–Kramers law for 1D SPDEs: comments

- Periodic b.c.: similar result [B & Gentz, Elec J Proba 2013]
  For $L > 2\pi$: extra factor $\sqrt{\varepsilon}$ because saddle is a whole curve
- Proof: relies on spectral Galerkin approximation ▸▸ Details
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  Details
- Similar results by F. Barret [Annales IHP, 2015]
  using different method (away from bifurcation points)
- For Neumann b.c. and $L < \pi$: spectral determinant in prefactor is explicitly computable (Euler product formulas)

$$\frac{1}{|\lambda_0|\nu_0}\prod_{k=1}^{\infty}\frac{\lambda_k}{\nu_k} = \frac{1}{2}\prod_{k=1}^{\infty}\frac{\left(\frac{k\pi}{L}\right)^2 - 1}{\left(\frac{k\pi}{L}\right)^2 + 2} = \frac{1}{2}\prod_{k=1}^{\infty}\frac{1 - \left(\frac{L}{k\pi}\right)^2}{1 + 2\left(\frac{L}{k\pi}\right)^2} = \frac{\sin(L)}{\sqrt{2}\sinh(\sqrt{2}L)}$$

  Similar expression for periodic b.c. and $L < 2\pi$
- For larger L, techniques for Feynman path integrals allow to compute the spectral determinants in prefactors [Maier & Stein]

The two-dimensional case

(Link to simulation)

The two-dimensional case

- Large-deviation principle: [Hairer & Weber, Ann. Fac. Sc. Toulouse, 2015]
- Naive computation of prefactor fails:

$$\log \prod_{k \in (\mathbb{N}^2)^*} \frac{1 - \left(\frac{L}{|k|\pi}\right)^2}{1 + 2\left(\frac{L}{|k|\pi}\right)^2} \simeq \sum_{k \in (\mathbb{N}^2)^*} \log\left(1 - \frac{3L^2}{|k|^2\pi^2}\right)$$

$$\simeq - \sum_{k \in (\mathbb{N}^2)^*} \frac{3L^2}{|k|^2\pi^2} \simeq -\frac{3L^2}{\pi^2} \int_1^\infty \frac{r\,\mathrm{d}r}{r^2} = -\infty$$

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$$\simeq -\sum_{k\in(\mathbb{N}^2)^*} \frac{3L^2}{|k|^2\pi^2} \simeq -\frac{3L^2}{\pi^2}\int_1^\infty \frac{r\,\mathrm{d}r}{r^2} = -\infty$$

- ▷ In fact, the equation needs to be renormalised

Theorem: [Da Prato & Debussche 2003]

Let ξ^δ be a mollification on scale δ of white noise. Then

$$\partial_t u = \Delta u + \left[1+\varepsilon C(\delta)\right]u - u^3 + \sqrt{2\varepsilon}\xi^\delta$$

with $C(\delta) \simeq \log(\delta^{-1})$ admits local solution converging as $\delta \to 0$.
(Global version: [Mourrat & Weber 2015])

Renormalisation

Problem: For $d = 2$, stoch. convolution $\int_0^t e^{\Delta(t-s)} \dot{W}_x(ds)$ is a distribution

- δ-mollification should be equivalent to Galerkin approx. $|k| \leqslant N = \delta^{-1}$:

$$w_N(x,t) = \sum_{|k| \leqslant N} a_k(t) \frac{1}{L} e^{i\Omega k \cdot x} \qquad a_k = \int_0^t e^{-\mu_k(t-s)} \, dW_s^{(k)}$$

$$\mu_k = (\Omega|k|)^2 \qquad \Omega = \beta\pi/L$$

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Problem: For $d = 2$, stoch. convolution $\int_0^t \mathrm{e}^{\Delta(t-s)} \dot{W}_x(\mathrm{d}s)$ is a distribution

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$$w_N(x,t) = \sum_{|k| \leqslant N} a_k(t) \frac{1}{L} \mathrm{e}^{\mathrm{i}\Omega k \cdot x} \qquad a_k = \int_0^t \mathrm{e}^{-\mu_k(t-s)} \mathrm{d}W_s^{(k)}$$

$$\mu_k = (\Omega|k|)^2 \qquad \Omega = \beta\pi/L$$

- $\lim_{t\to\infty} \int_0^t \mathrm{e}^{(\Delta-\mathbb{1})(t-s)} \dot{W}_x(\mathrm{d}s) = \phi_N$ is a Gaussian free field, s.t.

$$L^2 C_N := L^2 \mathbb{E}\phi_N^2 = \mathbb{E}\|\phi_N\|_{L^2}^2 = \sum_{|k| \leqslant N} \frac{1}{2(\mu_k + 1)} = \frac{\mathrm{Tr}(P_N[-\Delta + \mathbb{1}]^{-1})}{2} \simeq \log(N)$$

Renormalisation

Problem: For $d = 2$, stoch. convolution $\int_0^t e^{\Delta(t-s)} \dot{W}_x(ds)$ is a distribution

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▷ Wick powers

$$:\phi_N^2: = \phi_N^2 - C_N$$
$$:\phi_N^3: = \phi_N^3 - 3C_N\phi_N$$
$$:\phi_N^4: = \phi_N^4 - 6C_N\phi_N^2 + 3C_N^2$$

have zero mean and uniformly bounded variance

Computation of the prefactor

Work in progress with Giacomo Di Gesu and Hendrik Weber

- Consider for simplicity $L < \beta\pi \Rightarrow$ transition state in 0
- Galerkin-truncated renormalised potential

$$V_N = \frac{1}{2}\int_{\mathbb{T}^2}\left[u_N'(x)^2 - u_N(x)^2\right]\mathrm{d}x + \frac{1}{4}\int_{\mathbb{T}^2} :u_N(x)^4: \mathrm{d}x$$

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$$\int_{B^c} h_{A,B}(z)\,\mathrm{e}^{-V_N(z)/\varepsilon}\,\mathrm{d}z = \frac{1}{2}\int \mathrm{e}^{-V_N(z)/\varepsilon}\,\mathrm{d}z = \frac{1}{2}\mathcal{Z}_N(\varepsilon)$$

- $\mathcal{Z}_N(\varepsilon) \simeq 2\prod_{|k|\leqslant N}\sqrt{\frac{2\pi\varepsilon}{\nu_k}}\,\mathrm{e}^{-V_N(L,0)/\varepsilon}$ where $-V_N(L,0) = \frac{1}{4}L^2 + \frac{3}{2}L^2 C_N\varepsilon$

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- Prefactor proportionnal to (since $\nu_k = \lambda_k + 3$)

$$\prod_{0<|k|\leqslant N}\frac{\lambda_k}{\lambda_k+3}\mathrm{e}^{3/\lambda_k} \qquad \text{converges since} \qquad \log\Big[\frac{\lambda_k}{\lambda_k+3}\mathrm{e}^{3/\lambda_k}\Big] = \mathcal{O}\Big(\frac{1}{|k|^4}\Big)$$

Outlook

- ▷ Dim $d = 3$: more difficult because 2 renormalisation constants needed
- ▷ Potentials with more than two wells: essentially understood
- ▷ Potentials invariant under symmetry group: done for SDEs [5,6]
- ▷ Mainly open: non-gradient systems — But see poster by Manon Baudel

References: For this talk: [1,2,3]; Overview: [4]

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5. N. B. and Sébastien Dutercq, *The Eyring–Kramers law for Markovian jump processes with symmetries*, J. Theoretical Probability, First Online (2015)
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Sketch of proof: Spectral Galerkin approximation

$u_t^{(d)}(x) = \frac{1}{\sqrt{L}} \sum_{k=-d}^{d} z_k(t) \, \mathrm{e}^{\mathrm{i}\pi kx/L} \quad \Rightarrow \quad \mathrm{d}z_t = -\nabla V(z_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$

Theorem [Blömker & Jentzen 13]

For all $\gamma \in (0, \frac{1}{2})$ there exists an a.s. finite r.v. $Z : \Omega \to \mathbb{R}_+$ s.t. $\forall \omega \in \Omega$

$$\sup_{0 \leqslant t \leqslant T} \| u_t(\omega) - u_t^{(d)}(\omega) \|_{L^\infty} < Z(\omega) d^{-\gamma} \qquad \forall d \in \mathbb{N}$$

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Proposition (using potential theory)

$\exists \varepsilon_0 > 0$: $\forall \varepsilon < \varepsilon_0$ $\exists d_0(\varepsilon) < \infty$: $\forall d \geqslant d_0$ $\exists \nu_d$ proba measure on $\partial \mathcal{B}_r(u_-)$

$$\int_{\partial \mathcal{B}_r(u_-)} \mathbb{E}^{v_0}[\tau_+^{(d)}] \nu_d(dv_0) = C(d, \varepsilon) \, e^{H(d)/\varepsilon} \big[1 + R(\varepsilon) \big]$$

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Proposition (using large deviations and lots of other stuff)

$H_0 := V[u_{\text{ts}}] - V[u_-]$. $\forall \eta > 0$ $\exists \varepsilon_0, T_1, H_1$: $\forall \varepsilon < \varepsilon_0$ $\exists d_0 < \infty$ s.t. $\forall d \geqslant d_0$

$$\sup_{v_0 \in \mathcal{B}_r(u_-)} \mathbb{E}^{v_0}[\tau_+^2] \leqslant T_1^2\, e^{2(H_0+\eta)/\varepsilon}\ , \quad \sup_{d \geqslant d_0} \sup_{v_0 \in \mathcal{B}_r(u_-)} \mathbb{E}^{v_0}[(\tau_+^{(d)})^2] \leqslant T_1^2\, e^{2H_1/\varepsilon}$$

Main step of the proof

Set $T_{\mathrm{Kr}} = C(\infty, \varepsilon)\, \mathrm{e}^{H_0/\varepsilon}$

Let $B = \mathcal{B}_\rho(u_+)$ and define nested sets $B_- \subset B \subset B_+$ at L^∞-distance δ

$$\Omega_{K,d} = \left\{ \sup_{t \in [0, KT_{\mathrm{Kr}}]} \|v_t - v_t^{(d)}\|_{L^\infty} \leqslant \delta, \tau_{B_-}^{(d)} \leqslant KT_{\mathrm{Kr}} \right\}$$

$$\mathbb{P}(\Omega_{K,d}^c) \leqslant \mathbb{P}\{Z > \delta d^\gamma\} + \frac{\mathbb{E}^{v_0^{(d)}}[\tau_{B_-}^{(d)}]}{KT_{\mathrm{Kr}}} \quad \overset{\substack{\text{Cauchy–}\\ \text{Schwarz}}}{\Rightarrow} \quad \limsup_{d \to \infty} \mathbb{P}(\Omega_{K,d}^c) = \frac{M(\varepsilon)}{K}$$

Back

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$\Rightarrow$

$$\mathbb{E}^{v_0^{(d)}}[\tau_{B_+}^{(d)}] - \mathbb{E}^{v_0^{(d)}}[\tau_{B_+}^{(d)} 1_{\{\Omega_{K,d}^c\}}] \leqslant \mathbb{E}^{v_0}[\tau_B] \leqslant \mathbb{E}^{v_0^{(d)}}[\tau_{B_-}^{(d)}] + \mathbb{E}^{v_0}[\tau_B 1_{\{\Omega_{K,d}^c\}}]$$

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Integrate against ν_d and use Cauchy–Schwarz to bound error terms:
$\mathbb{E}^{v_0}[\tau_B 1_{\{\Omega_{K,d}^c\}}] \leqslant \sqrt{\mathbb{E}^{v_0}[\tau_B^2]\mathbb{P}(\Omega_{K,d}^c)}$, take $d \to \infty$ and finally K large

Back